Thermodynamic study of carbazole based hydrogen carriers for liquid hydrogen storage

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Improving hydrogen storage technology is a significant issue for the development of hydrogen economy. The compressed hydrogen gas tank has been developed as a commercialized storage technique, but it requires large amount of energy to compress hydrogen. Alternatively, Liquid Organic Hydrogen Carriers (LOHCs) such as cyclic hydrocarbons (e.g. toluene – methyl cyclohexane) or carbazole based compounds have been proposed as potential hydrogen storage materials. In this study, the reaction enthalpy for the dehydrogenation of carbazole-based compounds was calculated by Density Functional Theory and COnductor like Screening MOdel for Real Solvents method. In addition, hydrogenation reaction of proposed LOHCs was performed to verify its storage capacity. Product was analyzed by Nuclear Magnetic Resonance and Infrared spectroscopy. It was found that the complete dehydrogenation reaction of carbazole based compounds can occur at lower temperature compared with cyclic hydrocarbons. Also, hydrogen storage capacity raised above 6 wt%. These results provide that the proposed hydrogen storage candidates are economically feasible as a hydrogen carrier.